The realization of the technological promise of semiconductor nanoparticles requires a fundamental understanding of their nature and behavior. Recent research efforts have been focused on nanoscale semiconductors intentionally doped with magnetic impurities, i.e., quantum dots composed of dilute magnetic semiconductors (DMS’s). DMS quantum dots possess interesting properties owing to spin interactions enhanced by quantum confinement. I will present results for the electronic, magnetic and optical properties of Mn-doped group IV, III-V and II-VI semiconductor quantum dots using first-principles density-functional theory with pseudopotentials and real-space algorithms. A comparison of the electronic structures with that of bulk materials will be made and the confinement effect on the intrinsic properties of these nanostructures will be discussed.

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